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# A physically-based model for retrieving foliar biochemistry and leaf orientation using close-range imaging spectroscopy

Sylvain Jay<sup>a,\*</sup>, Ryad Bendoula<sup>a</sup>, Xavier Hadoux<sup>b,c</sup>, Jean-Baptiste Féret<sup>d</sup>, Nathalie Gorretta<sup>a</sup>

<sup>a</sup>Irstea, UMR ITAP, 361 rue J.F. Breton, 34196 Montpellier, France <sup>b</sup>Centre for Eye Research Australia, Royal Victorian Eye and Ear Hospital, Melbourne, Australia <sup>c</sup>Ophthalmology, University of Melbourne, Department of Surgery, Melbourne, Australia <sup>d</sup>Irstea, UMR TETIS, Maison de la Télédétection, 500 rue J.F. Breton, 34093 Montpellier, France

# Abstract

Radiative transfer models have long been used to characterize the foliar content at the leaf and canopy levels. However, they still do not apply well to close-range imaging spectroscopy, especially because directional effects are usually not taken into account. For this purpose, we introduce a physical approach to describe and simulate the variation in leaf reflectance observed at this scale. Two parameters are thus introduced to represent (1) specular reflection at the leaf surface and (2) local leaf orientation. The model, called COSINE (ClOse-range Spectral ImagiNg of lEaves), can be coupled with a directional-hemispherical reflectance model of leaf optical properties to relate

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<sup>\*</sup>Corresponding author at: Irstea, UMR ITAP, 361 rue J.F. Breton, 34196 Montpellier, France. Tel: +33467166459.

*E-mail addresses*: sylvain.jay@irstea.fr (S. Jay), ryad.bendoula@irstea.fr (R. Bendoula), xavier@hadoux.com (X. Hadoux), jean-baptiste.feret@teledetection.fr (J.B. Féret), nathalie.gorretta@irstea.fr (N. Gorretta).

the measured reflectance to the foliar content. In this study, we show that, when combining COSINE with the PROSPECT model, the overall PRO-COSINE model allows for a robust sub-millimeter retrieval of foliar content based on numerical inversion and pseudo bidirectional reflectance factor hyperspectral measurements.

The relevance of the added parameters is first shown through a sensitivity analysis performed in the visible and near-infrared (VNIR) and shortwave infrared (SWIR) ranges. PROCOSINE is then validated based on VNIR and SWIR hyperspectral images of various leaf species exhibiting different surface properties. Introducing these two parameters within the inversion allows us to obtain accurate maps of PROSPECT parameters, e.g., the chlorophyll content in the VNIR range, and the equivalent water thickness and leaf mass per area in the SWIR range. Through the estimation of light incident angle, the PROCOSINE inversion also provides information on leaf orientation, which is a critical parameter in vegetation remote sensing.

*Keywords:* close-range, COSINE, hyperspectral, imaging spectroscopy, leaf optical properties, pigment retrieval, PROCOSINE, PROSPECT, radiative transfer, vegetation

# 1 1. Introduction

Due to the strong interactions occurring between vegetation and the incoming optical radiation through absorption and scattering processes, hyperspectral remote sensing from satellites and aircrafts provides critical information to assess the spatial and temporal variabilities of vegetation status from local to global scales. This has led to a number of agricultural, envi-

ronmental and ecological applications such as the retrieval of leaf pigments 7 (Zarco-Tejada et al., 2004; Ustin et al., 2009), the early detection of leaf 8 diseases (Mahlein et al., 2013) or the mapping of forest biodiversity (Féret g & Asner, 2014). As hyperspectral cameras are now becoming more afford-10 able, close-range remote sensing data are also increasingly available to the 11 scientific community. Compared with air- and satellite-borne data, they gen-12 erally offer a sub-milliter or millimeter spatial resolution, and they can be 13 acquired at a higher temporal frequency, which is particularly interesting for 14 precision agriculture. For example, these data can be used to identify plant 15 pigments (Blackburn, 2007), freezing stress (Nicotra et al., 2003) or leaf dis-16 eases (Mahlein et al., 2013), each of which is of tremendous importance to 17 follow up the plant physiological status. These images are generally processed 18 by applying statistically-based methods to estimate various leaf biochemical 19 properties (Nicotra et al., 2003; Vigneau et al., 2011; Ji-Yong et al., 2012; Jay 20 et al., 2014). However, at this scale, a proper physical interpretation based 21 on radiative transfer modeling is needed to describe the interactions between 22 light and vegetation, especially for a spatially- and temporally-resolved quan-23 tification of pigments (Blackburn, 2007). 24

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Vegetation radiative transfer models are physically-based and simulate light propagation within leaves and/or canopies, e.g., as a function of leaf biochemical constituents, leaf anatomy or canopy structure. Whenever possible, model inversion allows for the retrieval of the variables of interest, generally using iterative optimization, look-up tables, statistical methods or machine learning algorithms.

At the leaf level, these models range from simple plate models, to ray-tracing, 32 radiosity and stochastic models that are computationally more difficult to in-33 vert (Dorigo et al., 2007). For instance, PROSPECT (Jacquemoud & Baret, 34 1990) is based on the generalized plate model, and is particularly well suited 35 to estimate leaf biochemical constituents (e.g., chlorophyll content, water 36 content and leaf mass per area) based on spectral measurements in the op-37 tical domain. The main reasons for the popularity of PROSPECT are its 38 accuracy, its computational efficiency (resulting in fast iterative model inver-39 sion) and free distribution. 40

At the canopy level, various approaches of different complexities have been developed for radiative transfer modeling, e.g., turbid medium approaches (Verhoef, 1984), geometrical approaches (Chen & Leblanc, 1997) or the combination of both (Gastellu-Etchegorry et al., 1996). Most of these models allow the canopy reflectance to be modeled as a function of parameters related to canopy structure (such as leaf area index or leaf inclination distribution function), leaf optical properties and sun-sensor geometry.

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However, leaf and canopy radiative transfer models do not apply well 49 to close-range imaging spectroscopy. For example, at the leaf level, the 50 directional-hemispherical reflectance and transmittance simulated by PROSPECT 51 (Jacquemoud & Baret, 1990) are usually measured with an integrating sphere, 52 whose implementation is difficult (if not impossible) for every single pixel of 53 hyperspectral images. As a result, PROSPECT cannot be inverted based on 54 directional reflectance data as retrieved by a close-range hyperspectral cam-55 era, unless it is assumed that leaves are Lambertian (Buddenbaum & Hill, 56

<sup>57</sup> 2015) and in fully horizontal position, which is an unrealistic hypothesis. <sup>58</sup> Indeed, in most cases, leaf reflectance exhibits some anisotropy (Bousquet <sup>59</sup> et al., 2005; Comar et al., 2012) and thus varies with respect to illumination <sup>60</sup> and viewing angles. Furthermore, variation in leaf orientation prevent from <sup>61</sup> achieving a proper reflectance correction for every pixel, because the refer-<sup>62</sup> ence surface used for reflectance correction is generally not submitted to the <sup>63</sup> same local illumination conditions than leaf material.

At the canopy level, most radiative transfer models have to be applied to 64 mixed pixels (containing both soil and leaf materials), for which effects of 65 leaf composition, canopy structure, soil properties and viewing/illumination 66 angles are integrated into a single spectrum. Canopy models are thus well 67 suited for ground-based spectroradiometric measurements, as well as for air-68 and satellite-borne hyperspectral measurements, all of them being usually 69 characterized by a spatial resolution coarser than one meter (Zarco-Tejada 70 et al., 2003; Colombo et al., 2008; Schlemmer et al., 2013). However, most 71 canopy models are not suitable for simulating hyperspectral data character-72 ized by a higher spatial resolution (up to sub-millimeter level) for which the 73 assumption of mixed pixel does not hold. 74

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In this study, we propose a physically-based model, called COSINE (ClOserange Spectral ImagiNg of lEaves), that describes the additional spectral variability induced by directional effects and variation in leaf orientation. Combining COSINE with a leaf directional-hemispherical reflectance model such as PROSPECT allows the simulation of leaf reflectance according to our experimental conditions: submillimetric spatial resolution and a single

<sup>82</sup> light source assumed to be directional. When applied in inverse mode to <sup>83</sup> close-range hyperspectral images, the overall PROCOSINE model enables <sup>84</sup> the simultaneous retrieval of PROSPECT parameters (e.g., chlorophyll and <sup>85</sup> water contents), bidirectional effects and leaf angle with respect to the light <sup>86</sup> source.

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The COSINE theory is described in Section 2. After recalling the nec-88 essary radiometric definitions, we develop a physically-based analytic ex-89 pression of the reflectance quantity retrieved using close-range imaging spec-90 troscopy. This expression is then related to PROSPECT to explain variations 91 in leaf biochemistry and leaf anatomy. In Section 3, we present the data sets 92 used in this article as well as details about model validation and sensitivity 93 analysis. Results are presented and discussed in Section 4, and we finally 94 draw some conclusions and perspectives in Section 5. 95

# 96 2. Theory

# 97 2.1. Radiometric considerations

98 2.1.1. Definitions

The definitions and notations of the main physical quantities used in this article and summarized in Table 1, are based on the initial terminology of Nicodemus et al. (1977), which has later been reviewed by Schaepman-Strub et al. (2006).

<sup>103</sup> The spectral radiance L is the radiant flux in a beam per unit wavelength, <sup>104</sup> per unit area and per unit solid angle, and is expressed in the SI unit <sup>105</sup> [W.sr<sup>-1</sup>.m<sup>-2</sup>.nm<sup>-1</sup>]. This is the physical quantity measured by a hyper-

Parameter	Definition [unit]
$b_{spec}$	Specular term [unitless]
$C_{ab}$	Chlorophyll a+b content $[\mu g.cm^{-2}]$
$C_{bp}$	Brown pigment content [unitless]
$C_{cx}$	Carotenoid content $[\mu g.cm^{-2}]$
$C_m$	Leaf mass per area $[g.cm^{-2}]$
$C_w$	Equivalent water thickness [cm]
E	Spectral irradiance $[W.m^{-2}.nm^{-1}]$
$f_r$	Bidirectional reflectance distribution function (BRDF) $[sr^{-1}]$
L	Spectral radiance $[W.sr^{-1}.m^{-2}.nm^{-1}]$
$\lambda$	Wavelength [nm]
N	Leaf structure parameter [unitless]
$arphi_l$	Difference between illumination and leaf normal azimuth angles $\left[^o\right]$
$\varphi_v$	Difference between illumination and viewing azimuth angles $\left[^o\right]$
R	Bidirectional reflectance factor (BRF) [unitless]
$R_{hsi}$	Pseudo bidirectional reflectance factor [unitless]
ρ	Directional-hemispherical reflectance (DHR) [unitless]
$ heta_i$	Light incident angle (angle between the light source and the normal
	to the leaf) $[^{o}]$
$\theta_l,\theta_v,\theta_s$	Leaf normal, viewing and illumination zenith angles $\left[^o\right]$
θ	PROCOSINE parameters
$oldsymbol{artheta}_{dhr}$	Parameters of the leaf DHR model

Table 1: Main parameters and acronyms.

<sup>106</sup> spectral imaging sensor after spectral calibration. The spectral irradiance E<sup>107</sup> is the radiant flux in a beam per unit wavelength and per unit area and is <sup>108</sup> expressed in [W.m<sup>-2</sup>.nm<sup>-1</sup>].

One of the main physical quantities used to describe angular patterns of reflected light is the bidirectional reflectance distribution function (BRDF) expressed in  $[sr^{-1}]$ . It describes how a parallel beam of incident light from one direction in the hemisphere is reflected into another direction in the hemisphere:

$$f_r(\theta_s; \theta_v, \varphi_v; \lambda) = \frac{dL_r(\theta_s; \theta_v, \varphi_v; \lambda)}{dE_i(\theta_s; \lambda)}$$
(1)

where subscripts *i* and *r* refer to incoming and reflected lights respectively,  $\theta_s$  and  $\theta_v$  are respectively the illumination and viewing zenith angles, and  $\varphi_v$  is the viewing azimuth angle relatively to the illumination azimuth angle (see Fig. 1 for angle representation). The BRDF being the ratio of two infinitesimal quantities, it cannot theoretically be measured. However, its integration over the corresponding solid angles allows the derivation of many other measurable physical quantities.

Usually, the reflectance correction process does not consist in retrieving di-121 rectly the reflectance (defined as the ratio of the leaving radiant exitance 122 to the incident irradiance), but rather follows the definition of a reflectance 123 factor. In the specific case of single illumination and viewing directions, the 124 bidirectional reflectance factor (BRF, denoted by R) is given by the ratio of 125 the radiant flux  $dL_r$  reflected from the area element dA to the radiant flux 126  $dL_r^{id}$  reflected from an ideal and diffuse surface of the same area dA under 127 identical illumination and viewing geometries. It is unitless and, as developed 128



Figure 1: Angle representation.

<sup>129</sup> by Schaepman-Strub et al. (2006), it can be expressed as follows:

$$R(\theta_s; \theta_v, \varphi_v; \lambda) = \frac{dL_r(\theta_s; \theta_v, \varphi_v; \lambda)}{dL_r^{id}(\theta_s; \lambda)}$$
(2)

where  $dL_r^{id}$  does not depend on viewing angles because of the Lambertian nature of the reference surface.

The BRDF of an ideal and diffuse surface being  $(1/\pi)$ , the BRF of any surface is therefore related to its BRDF by:

$$R(\theta_s; \theta_v, \varphi_v; \lambda) = \pi f_r(\theta_s; \theta_v, \varphi_v; \lambda).$$
(3)

Let us finally define the directional-hemispherical reflectance (DHR) as the integration of BRDF over the whole viewing hemisphere. The DHR is unitless and is given by:

$$\rho(\theta_s; 2\pi; \lambda) = \int_0^{2\pi} \int_0^{\pi/2} f_r(\theta_s; \theta_v, \varphi_v; \lambda) \cos \theta_v \sin \theta_v d\theta_v d\varphi_v.$$
(4)

In the following, the spectral dependence will be omitted for more clarity in
notation. Similarly, spectral radiance and spectral irradiance will be simply
referred to as radiance and irradiance.

#### <sup>140</sup> 2.1.2. Radiometric expression of close-range hyperspectral measurement

The solid angles corresponding to incident and reflected light beams are 141 never purely directional, so rigorously, sensor measurements only allow the 142 retrieval of a biconical reflectance factor (Schaepman-Strub et al., 2006). 143 However, a close approximation of bidirectional reflectance can be obtained 144 under specific experimental and instrumental conditions, e.g., using a col-145 limited light beam and a small sensor field of view (FOV) provided by a 146 push-broom hyperspectral camera. In this case, the leaf BRF R is approxi-14 mated as follows: 148

$$R(\theta_s; \theta_v, \varphi_v) \approx \frac{L_r(\theta_s; \theta_v, \varphi_v)}{L_r^{id}(\theta_s)}$$
(5)

where  $L_r$  and  $L_r^{id}$  are the radiances respectively measured on the leaf and on the reference surface with a hyperspectral camera.

Importantly, Eq. 5 requires the leaf and reference surface to be under identical illumination geometry (i.e., same  $\theta_s$  values). However, at the pixel level, the leaf position and leaf local orientation can make the irradiances received by the leaf and reference surface strongly different. Indeed, considering a directional light source, the irradiance received by an area element is proportional to the cosine of the incident angle  $\theta_i$ , i.e., the angle between the light source and the normal to this element:

$$E_i(\theta_i) = E_0 \cos \theta_i \tag{6}$$

where  $E_0$  is the irradiance received by an area element perpendicular to the light source direction, and  $\cos \theta_i = \cos \theta_s \cos \theta_l + \sin \theta_s \sin \theta_l \cos \varphi_l$  where  $\theta_l$ and  $\varphi_l$  characterize the normal to this area element (Bousquet et al., 2005; Comar et al., 2014).

Therefore, we define two illumination geometries corresponding to either the
leaf or the reference surface. The irradiance received by the leaf is:

$$E_i^l(\theta_i^l) = E_0 \cos \theta_i^l \tag{7}$$

<sup>164</sup> whereas the one received by the ideal and diffuse reference surface is:

$$E_i^{id}(\theta_i^{id}) = E_0 \cos \theta_i^{id}.$$
(8)

The reference surface is usually positioned horizontally so, in the following, we note  $\theta_i^{id} = \theta_s$  and  $\theta_i^l = \theta_i$ .

Similarly to Eq. 5, at each pixel, the physical quantity  $R_{hsi}$  retrieved using a hyperspectral camera is given by:

$$R_{hsi}(\theta_s, \theta_i; \theta_v, \varphi_v) \approx \frac{L_r(\theta_i; \theta_v, \varphi_v)}{L_r^{id}(\theta_s)}.$$
(9)

Assuming the light source is directional and the pixel FOV is small, combining Eq. 1 and Eq. 9 leads to the following equation:

$$R_{hsi}(\theta_s, \theta_i; \theta_v, \varphi_v) \approx \frac{f_r(\theta_i; \theta_v, \varphi_v) E_i^l(\theta_i)}{(1/\pi) E_i^{id}(\theta_s)}.$$
 (10)

Using Eq. 3, Eq. 7 and Eq. 8,  $R_{hsi}$  can finally be expressed as follows:

$$R_{hsi}(\theta_s, \theta_i; \theta_v, \varphi_v) \approx R(\theta_i; \theta_v, \varphi_v) \frac{\cos \theta_i}{\cos \theta_s}.$$
 (11)

<sup>172</sup> Eq. 11 reveals that the physical reflectance quantity retrieved from a small <sup>173</sup> FOV sensor in presence of a directional light source does not correspond

to the leaf BRF if the leaf and reference surface are differently tilted with 174 respect to the light source. In the following, we call "leaf pseudo BRF" the 175 leaf BRF weighted by the ratio of the cosine of the angle between the light 176 source and the normal to the leaf, to the cosine of illumination zenith angle. 17 Therefore, Eq. 11 relates the measured leaf pseudo BRF to the illumination 178 zenith angle, the incident angle (related to local leaf angles and illumination 179 zenith angle) and the leaf BRF. To relate the latter to the foliar content, it 180 is then necessary to take into account leaf surface properties as described in 181 the next section. 182

# <sup>183</sup> 2.2. COSINE: a model for ClOse-range Spectral ImagiNg of lEaves

In this study, we propose to adapt a leaf DHR model (such as PROSPECT 184 (Jacquemoud & Baret, 1990) or LIBERTY (Dawson et al., 1998)) to the close-185 range case. Indeed, with the perspective of comparing leaf optical measure-186 ments to DHR simulations, proper experimental acquisitions require using an 18 integrating sphere in order to match with the hemispherical simulations. As 188 a result, leaf DHR models cannot directly be applied to hyperspectral remote 189 sensing observations of vegetation that are affected by variable bidirectional 190 effects (or BRDF effects) depending on illumination and viewing geometries. 19 An important prerequisite before using these models for close-range imaging 192 spectroscopy, is therefore to relate the leaf DHR to the leaf BRDF. 193

#### <sup>194</sup> 2.2.1. Relationship between leaf BRDF and DHR

It is generally admitted that the leaf BRDF is the sum of a diffuse component  $f_{r,diff}$  and a directional component  $f_{r,spec}$  (Bousquet et al., 2005; Comar

<sup>197</sup> et al., 2014):

$$f_r(\theta_i; \theta_v, \varphi_v) = f_{r,spec}(\theta_i; \theta_v, \varphi_v) + f_{r,diff}(\theta_i; \theta_v, \varphi_v).$$
(12)

The diffuse component  $f_{r,diff}$  characterizes absorption and scattering pro-198 cesses within the leaf volume and thus depends on optically-active biochemi-199 cal and biophysical parameters. The directional component  $f_{r,spec}$  character-200 izes leaf surface properties and describes how light is reflected at the surface. 201 While  $f_{r,diff}$  is strongly wavelength-dependent,  $f_{r,spec}$  is assumed to be nearly 202 wavelength-independent in the visible and near-infrared (VNIR) range (be-203 tween 400 and 1000 nm) (Bousquet et al., 2005; Comar et al., 2014). In 204 the shortwave infrared (SWIR) range (between 1000 and 2500 nm), this as-205 sumption does not hold because the leaf refractive index actually depends on 206 wavelength (Féret et al., 2008; Vanderbilt & Grant, 1985), especially due to 20 the non-negligible influence of water absorption. 208

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As a first approximation,  $f_{r,diff}$  can be expressed as the ratio of leaf 210 mesophyll Lambert coefficient  $k_l$  to  $\pi$  (Bousquet et al., 2005). To take into 211 account the two-layer leaf structure (i.e. composed of an upper wax layer and 212 a bottom leaf mesophyll layer), one should also consider the fraction of light 213 that is reflected by the first wax layer and that does not reach the bottom 214 layer (Stuckens et al., 2009; Ashikmin et al., 2000). The diffuse component 215 is then expressed as a function of leaf mesophyll Lambert coefficient  $k_l$  and 216 wax DHR  $\rho_{spec}$  (Stuckens et al., 2009): 217

$$f_{r,diff}(\theta_i) = \frac{k_l}{\pi} (1 - \rho_{spec}(\theta_i; 2\pi))$$
(13)

where  $f_{r,diff}$  does not depend on viewing angles and  $k_l$  only depends on

wavelength.

As defined by Eq. 4, the total DHR can then be obtained combining Eq. 12 and Eq. 13:

$$\rho(\theta_i; 2\pi) = \int_0^{2\pi} \int_0^{\pi/2} f_{r,spec}(\theta_i; \theta_v, \varphi_v) \cos \theta_v \sin \theta_v d\theta_v d\varphi_v + \frac{k_l}{\pi} (1 - \rho_{spec}(\theta_i; 2\pi)) \int_0^{2\pi} \int_0^{\pi/2} \cos \theta_v \sin \theta_v d\theta_v d\varphi_v \quad (14)$$

<sup>218</sup> which can be rewritten as follows:

$$\rho(\theta_i; 2\pi) = \rho_{spec}(\theta_i; 2\pi) + k_l(1 - \rho_{spec}(\theta_i; 2\pi)).$$
(15)

This equation provides the necessary basis to relate a leaf DHR model to theleaf BRDF (through the Lambert coefficient).

221 2.2.2. The COSINE model

Assuming nadir illumination, a leaf DHR model expresses the DHR  $\rho(0; 2\pi)$ as a function of leaf biochemical and biophysical contents characterized by the vector of input parameters  $\boldsymbol{\vartheta}_{dhr}$ . Following Eq. 15, the modeled Lambert coefficient can be expressed as a function of  $\rho_{spec}(0; 2\pi)$  and DHR model  $\widetilde{\rho}(\boldsymbol{\vartheta}_{dhr})$  as:

$$\widetilde{k}_{l}(\boldsymbol{\vartheta}_{dhr}) = \frac{\widetilde{\rho}(\boldsymbol{\vartheta}_{dhr}) - \rho_{spec}(0; 2\pi)}{1 - \rho_{spec}(0; 2\pi)}$$
(16)

where  $\widetilde{\phantom{\alpha}}$  refers to modeled quantities.

The leaf BRDF can then be modeled as a function of leaf parameters  $\vartheta_{dhr}$  by combining Eq. 12, Eq. 13 and Eq. 16:

$$f_r(\theta_i; \theta_v, \varphi_v; \boldsymbol{\vartheta}_{dhr}) = f_{r,spec}(\theta_i; \theta_v, \varphi_v) + \frac{1}{\pi} \left( \frac{1 - \rho_{spec}(\theta_i; 2\pi)}{1 - \rho_{spec}(0; 2\pi)} \right) (\widetilde{\rho}(\boldsymbol{\vartheta}_{dhr}) - \rho_{spec}(0; 2\pi)).$$
(17)

In order to estimate  $\vartheta_{dhr}$  from the pseudo BRF  $R_{hsi}$  retrieved using a hyperspectral camera, Eq. 3, Eq. 11 and Eq. 17 are combined to obtain the pseudo-BRF based COSINE model:

$$\widetilde{R_{hsi}}(\theta_s, \theta_i; \theta_v, \varphi_v; \boldsymbol{\vartheta}_{dhr}) = \left(\frac{\cos \theta_i}{\cos \theta_s}\right) \left[ \left(\frac{1 - \rho_{spec}(\theta_i; 2\pi)}{1 - \rho_{spec}(0; 2\pi)}\right) \widetilde{\rho}(\boldsymbol{\vartheta}_{dhr}) + \pi f_{r,spec}(\theta_i; \theta_v, \varphi_v) - \rho_{spec}(0; 2\pi) \left(\frac{1 - \rho_{spec}(\theta_i; 2\pi)}{1 - \rho_{spec}(0; 2\pi)}\right) \right]$$
(18)

<sup>227</sup> where only the first term of the sum is related to the leaf DHR model.

Note that  $f_{r,spec}$  and  $\rho_{spec}$  could potentially be modeled using the leaf BRDF model developed by Bousquet et al. (2005) that expresses the directional component as a function of illumination and viewing geometries as well as on the wax refractive index and a surface roughness parameter. Unfortunately, the resulting model becomes over-parameterized so its inversion is an ill-posed problem and leads to poor estimation results (not shown).

# 234 2.2.3. A simplified COSINE model for the VNIR range

In the VNIR range, the second term in Eq. 18 is assumed to be wavelengthindependent. Omitting its dependence in viewing angles, Eq. 18 can then be simplified as:

$$\widetilde{R_{hsi}}(\theta_s, \theta_i; \boldsymbol{\vartheta}_{dhr}, b_{spec}) = \left(\frac{\cos \theta_i}{\cos \theta_s}\right) \left[ \left(\frac{1 - \rho_{spec}(\theta_i; 2\pi)}{1 - \rho_{spec}(0; 2\pi)}\right) \widetilde{\rho}(\boldsymbol{\vartheta}_{dhr}) + b_{spec} \right]$$
(19)

where  $b_{spec} = b_{spec}(\theta_i; \theta_v, \varphi_v) = \pi f_{r,spec}(\theta_i; \theta_v, \varphi_v) - \rho_{spec}(0; 2\pi) \left(\frac{1 - \rho_{spec}(\theta_i; 2\pi)}{1 - \rho_{spec}(0; 2\pi)}\right)$ . Assuming that the fraction  $\frac{1 - \rho_{spec}(\theta_i; 2\pi)}{1 - \rho_{spec}(0; 2\pi)}$  is nearly one (especially true for low incident angles), Eq. 19 can be approximated by:

$$\widetilde{R_{hsi}}(\theta_s, \theta_i; \boldsymbol{\vartheta}_{dhr}, b_{spec}) = \left(\frac{\cos \theta_i}{\cos \theta_s}\right) \left[\widetilde{\rho}(\boldsymbol{\vartheta}_{dhr}) + b_{spec}\right].$$
 (20)

COSINE therefore simulates the pseudo-BRF as a function of incident angle  $\theta_i$ , illumination zenith angle  $\theta_s$ , foliar content through the DHR model parameters  $\boldsymbol{\vartheta}_{dhr}$  and BRDF effect  $b_{spec}$ . Importantly, this model is presumably only well suited for low incident angles. In high incidence, the fraction  $\frac{1-\rho_{spec}(\theta_i;2\pi)}{1-\rho_{spec}(0;2\pi)}$  may differ from one, which could lead to an incorrect estimation of  $\theta_i$  when inverting the model.

Finally, in order to model directly radiance measurements, a radiance-based
COSINE model can be derived from Eq. 9 as:

$$\widetilde{L_r}(\theta_s, \theta_i; \boldsymbol{\vartheta}_{dhr}, b_{spec}) = \left(\frac{\cos \theta_i}{\cos \theta_s}\right) \left[\widetilde{\rho}(\boldsymbol{\vartheta}_{dhr}) + b_{spec}\right] L_r^{id}(\theta_s)$$
(21)

where  $L_r^{id}(\theta_s)$  is the radiance measured on the reference surface.

# <sup>250</sup> 3. Material and methods

# 251 3.1. Data acquisition

### 252 3.1.1. Spectral measurements

The COSINE model was tested using close-range hyperspectral images 253 acquired under laboratory conditions. Two push-broom hyperspectral cam-254 eras were used, i.e., a HySpex VNIR-1600 camera (Norsk Elektro Optikk, 255 Norway) and a HySpex SWIR-320m-e camera (Norsk Elektro Optikk, Nor-256 way). The HySpex VNIR-1600 camera acquired successive lines of 1600 pixels 25 and 160 spectral bands ranging from 415 to 994 nm with a 3.7 nm spectral 258 sampling interval. The pixel FOV was 0.18 and 0.36 mrad across- and along-250 track respectively. 260

Even if COSINE is theoretically only well suited for the VNIR range for which
the directional BRDF component is assumed to be wavelength-independent,



Figure 2: Experimental setup for the horizontal (a) and tilted (b-c) configurations. For the VNIR camera, the corresponding average incident angles  $\bar{\theta}_i$  are 20° (a), 40° (b) and 0° (c). For the SWIR camera, the corresponding average incident angles  $\bar{\theta}_i$  are 30° (a), 10° (b) and 50° (c).

we also tested this model on SWIR images in order to see how this assumption was affecting the estimation results. The HySpex SWIR-320m-e camera acquired successive lines of 320 pixels and 256 spectral bands ranging from 960 to 2490 nm with a 6 nm spectral sampling interval. The pixel FOV was 0.75 mrad across- and along-track.

As shown in Fig. 2, in both cases, the camera was facing towards nadir at thirty centimeters above the imaged leaf, thus leading to across-track pixel FOV of 0.23 mm for the SWIR camera, and 0.11 mm for the VNIR camera (after an appropriate subsampling in the across-track direction so as to obtain square pixels). Both cameras were positioned thirty centimeters apart. The lighting was provided by two halogen sources (one for each camera) positioned close to the cameras. These light sources were collimated and

positioned so that each source was illuminating the same line than the line 275 imaged by the corresponding camera. The illumination zenith angles were 276 set to  $\theta_s = 20^o$  and  $\theta_s = 30^o$  for the VNIR camera and the SWIR camera 27 respectively. The incoming halogen irradiance was estimated on a line-by-278 line basis by using a reference surface (Spectralon<sup>®</sup>, Labsphere) horizontally 279 placed next to the imaged leaf. In order to limit saturation on the reference 280 surface while obtaining a low noise level in the strong absorption regions, 28 we chose a Spectralon<sup>®</sup> whose diffuse reflectance was approximately 40% 282 between 400 and 2500 nm. After acquisition, VNIR and SWIR images were 283 finally calibrated to spectral radiance. 284

285

The main data set contains leaves from five species commonly found in 286 the French Mediterranean region, namely bamboo (*Phyllostachys aurea*), ivy 28 (Hedera helix), laurestine (Viburnum tinus), bay laurel (Laurus nobilis) and 288 holly (*Ilex aquifolium*). Some of these leaves exhibited strong (resp. weak) 280 non-Lambertian behavior, e.g., bay laurel and holly (resp. bamboo). Also, 290 some of them had regular (resp. non-regular) surfaces, e.g., bay laurel (resp. 29 ivy and holly). All of these leaves were harvested in March, 2015 and selected 292 on a color basis, ranging from dark green for leaves with a high chlorophyll 293 content, to yellow for senescent leaves. As illustrated in Fig. 2, each leaf was 294 placed on a translation stage and was imaged in three positions using a  $20^{\circ}$ 295 tilted stand. As a result, the average incident angles  $\bar{\theta}_i$  were 0°, 20° and 296  $40^{\circ}$  for VNIR camera, and  $10^{\circ}$ ,  $30^{\circ}$  and  $50^{\circ}$  for SWIR camera. Note that 29 the translation stage had low reflectivity so we assumed that, after being 298 transmitted through the leaf, the light reflected from the translation stage 290

<sup>300</sup> and re-transmitted through the leaf was negligible.

In addition, a SWIR image of a sugar beet leaf (*Beta vulgaris*) was acquired, especially because this species shows interesting features in this spectral range, i.e., very high equivalent water thickness ( $C_w > 0.02$  cm) and low leaf mass per area ( $C_m < 0.005$  g.cm<sup>-2</sup>), as well as a strongly non-Lambertian and non-regular surface, thereby illustrating well the relevance of our model. This leaf was only imaged in horizontal position, its surface being already highly non-regular.

#### 308 3.1.2. Reference measurements

For each leaf, after spectral measurements, several leaf disks (from two to 309 seven disks depending on leaf size) of known area were sampled using a cork 310 borer. Each disk position was then recorded for further reference. A Dualex 31 scientific+<sup>TM</sup> (Force-A, Orsay, France), hereafter called Dualex, was used to 312 measure the chlorophyll a+b content  $C_{ab}$  in every disk. This leafclip allows 313 non-destructive transmittance-based  $C_{ab}$  measurements characterized by an 314 accuracy of around 5  $\mu$ g.cm<sup>-2</sup> (Cerovic et al., 2012). Compared with the well 315 known SPAD-502<sup>TM</sup> (Minolta, Japan), the Dualex uses a higher  $C_{ab}$ -sensitive 316 wavelength (710 nm) that allows it to have a nearly linear response to vari-31 ation in  $C_{ab}$  for  $C_{ab} < 40 \ \mu g.cm^{-2}$ . However, for dicotyledons, saturation 318 occurring beyond 40  $\mu g.cm^{-2}$  leads the Dualex to underestimate such  $C_{ab}$ 319 values (Cerovic et al., 2012). The higher  $C_{ab}$ , the greater the underestima-320 tion. 321

Leaf disks were then weighted and placed in a drying oven at 75°C for 48 h. Subsequently, their dry mass was measured to obtain the equivalent water

Table 2: Characteristics of reference measurements for the main data set.ParameterNumber of samplesMeanMin/MaxStandard deviation

Parameter	Number of samples	Mean	Min/Max	Standard deviation
$C_{ab} \ [\mu \mathrm{g.cm^{-2}}]$	93	29.4	5.2/54.6	11.1
$C_w$ [cm]	22	0.0104	0.0049/0.0164	0.0040
$C_m  [\mathrm{g.cm}^{-2}]$	22	0.0091	0.0052/0.0129	0.0023

thickness  $C_w$  (in [cm]) and leaf mass per area  $C_m$  (in [g.cm<sup>-2</sup>]) as follows:

$$C_w = \frac{FW - DW}{A} \times d_w \tag{22}$$

$$C_m = \frac{DW}{A} \tag{23}$$

where FW and DW are the fresh and dry weights of leaf disks respectively, A is the total disk area, and  $d_w = 1 \text{ g.cm}^{-3}$  is the water density.

Therefore, for each leaf, several measurements of  $C_{ab}$  and one measurement of  $C_w$  and  $C_m$  were available. The ranges of  $C_{ab}$ ,  $C_w$  and  $C_m$  for the main data set are reported in Table 2 and were similar to those found in the literature (Féret et al., 2008; Danson & Bowyer, 2004).

#### 331 3.2. Retrieval of leaf parameters from model inversion

In this study, we used the PROSPECT (Leaf Optical Properties Spectra) 332 model to simulate the leaf DHR from 400 to 2500 nm as a function of the leaf 333 biochemistry and structure. The original version developed by Jacquemoud 334 & Baret (1990) has been successively improved over the years to take into 335 account other biochemical components and a broader spectral range (Jacque-336 moud et al., 1996; Baret & Fourty, 1997a; Jacquemoud et al., 2000; Féret 33 et al., 2008; Gerber et al., 2011). The considered PROSPECT 5b version was 338 developed by Féret et al. (2008) (available at http://teledetection.ipgp. 339

jussieu.fr/prosail/) and simulates the leaf DHR as a function of the leaf structure parameter N, chlorophyll a+b content  $C_{ab}$ , carotenoid content  $C_{cx}$ , brown pigment content  $C_{bp}$ , equivalent water thickness  $C_w$  and leaf mass per area  $C_m$ .

In the following, leaf parameters were retrieved based on model inversion. 344 The parameters that were only affecting the reflected radiation in the VNIR 345 range (resp. the SWIR range), were kept constant when considering the 346 SWIR range (resp. the VNIR range) so as to reduce the estimation un-34 certainty. Therefore, because water absorption is weak in the VNIR range 348 and only occurs around 970 nm (Curran, 1989), the VNIR range was re-349 duced to 410-900 nm (i.e., 135 bands) and  $C_w$  was fixed to the default value 350 0.01 cm. The vector of input PROSPECT parameters was thus  $\vartheta_{dhr} =$ 35  $[N, C_{ab}, C_{cx}, C_{bp}, C_m]^t$ . Similarly, foliar pigments do not affect the SWIR re-352 flectance so  $C_{ab}$ ,  $C_{cx}$  and  $C_{bp}$  were fixed to the default values 30  $\mu$ g.cm<sup>-2</sup>, 353 10  $\mu$ g.cm<sup>-2</sup> and 0 respectively. In the SWIR range, the vector of input 354 PROSPECT parameters was  $\boldsymbol{\vartheta}_{dhr} = [N, C_w, C_m]^t$ . 355

For each pixel, the combined pseudo-BRF based PROSPECT+COSINE model (named PROCOSINE hereafter) was numerically inverted by optimizing the following least square merit function:

$$\widehat{\boldsymbol{\vartheta}}_{pseudo-brf} = \underset{\boldsymbol{\vartheta}}{\operatorname{argmin}} \sum_{\lambda_i} \left[ R_{hsi}(\lambda_i) - \widetilde{R_{hsi}}(\lambda_i; \boldsymbol{\vartheta}) \right]^2$$
(24)

where  $\boldsymbol{\vartheta} = [\boldsymbol{\vartheta}_{dhr}, \theta_i, b_{spec}]^t$ ,  $R_{hsi}$  is the measured pseudo-BRF retrieved using Eq. 9 and  $\widetilde{R_{hsi}}$  is the pseudo-BRF based PROCOSINE model given by Eq. 20. Similarly, the radiance-based PROCOSINE model was inverted by solving

Parameter	Lower bound	Upper bound	Initial value
N	1	3.5	1.5
$C_{ab} \ [\mu \mathrm{g.cm^{-2}}]$	0	100	50
$C_{cx} \; [\mu \mathrm{g.cm}^{-2}]$	0	30	10
$C_{bp}$	0	5	0
$C_w$ [cm]	0.00005	0.1	0.01
$C_m  [\mathrm{g.cm}^{-2}]$	0.001	0.03	0.01
$ heta_i ~[^o]$	0	90	20
$b_{spec}$	-0.2	0.6	0

Table 3: Lower bounds, upper bounds and initial values of the optimization problem.

#### <sup>362</sup> the following optimization problem:

$$\widehat{\boldsymbol{\vartheta}}_{radiance} = \underset{\boldsymbol{\vartheta}}{\operatorname{argmin}} \sum_{\lambda_i} \left[ L_r(\lambda_i) - \widetilde{L_r}(\lambda_i; \boldsymbol{\vartheta}) \right]^2$$
(25)

where  $L_r$  is the measured spectral radiance and  $\widetilde{L_r}$  is the radiance-based PROCOSINE model given by Eq. 21.

365

To reduce the number of solutions to the inverse problem, the estimation 366 range was restricted using lower and upper bounds. These bounds as well as 367 initial values are provided in Table 3. Note that  $C_{bp}$  and  $C_w$  upper bounds 368 are higher than those found in the literature because, at the sub-millimeter 369 level,  $C_{bp}$  and  $C_w$  can be very high in necrotic regions and veins respectively. 370 Optimization of Eq. 24 and Eq. 25 was performed using the trust-region 371 reflective algorithm implemented in MATLAB<sup>®</sup> (version 8.0.0, The Math-372 Works Inc., Natick, MA, 2012) within the "lsqcurvefit" function. 373

#### 374 3.3. PROCOSINE sensitivity analysis

Before assessing PROCOSINE in terms of estimation results, we per-375 formed a global sensitivity analysis in order to study the relative contribution 376 of each parameter to the modeled pseudo-BRF as a function of wavelength. 37 Global sensitivity analysis informs us on which variation in the model output 378 is produced by variation in the model input parameters, both individually 379 and collectively through their interactions with each other. When studied as 380 a function of wavelength, it provides interesting insights regarding the opti-38 mal spectral bands that can be used to retrieve model parameters. 382

383

In this paper, we implemented the EFAST (Extended Fourier Amplitude 384 Sensitivity Transform) method (Saltelli et al., 1999) that was already ap-385 plied to PROSAIL and PROGEOSAIL models by Bowyer & Danson (2004). 386 EFAST is a quantitative variance-based method, i.e., it allows the deriva-38 tion of sensitivity indices from the decomposition of the total variance of the 388 model output into variance terms induced by every input parameter. In this 389 paper, we only used the first-order index  $S_i$  that represents the percentage 390 of output variance explained by the i<sup>th</sup> parameter alone. The remaining per-39 centage of variance is explained by interactions between parameters and is 392 given by  $S_{int} = 1 - \sum_{i} S_i$ .  $S_i$  (and  $S_{int}$ ) ranges from 0 to 1, and the higher 393  $S_i,$  the more sensitive the model output is to the  $\mathbf{i}^{\mathrm{th}}$  parameter. 394 395

In this study, 5000 combinations of model parameters were randomly generated using appropriate probability distributions because the latter strongly affects the results of sensitivity analysis (Bowyer & Danson, 2004; Wallach

Parameter	Distribution	$\mu$	σ	α	$\beta$
N	Gamma	1.52	0.23	47.50	0.032
$C_{ab} \ [\mu \mathrm{g.cm^{-2}}]$	Gamma	32.8	18.87	1.99	16.45
$C_{cx} \; [\mu \mathrm{g.cm}^{-2}]$	Gamma	8.51	3.92	3.83	2.22
$C_w$ [cm]	Gamma	0.0122	0.0061	6.45	0.0019
$C_m  [\mathrm{g.cm}^{-2}]$	Gamma	0.0078	0.0036	4.20	0.0018
$ heta_i ~[^o]$	Gamma	25	10	6.25	4
$b_{spec}$ (VNIR)	Normal	-0.009	0.0375	-	-
$b_{spec}$ (SWIR)	Normal	0.0346	0.0403	-	-

Table 4: Estimated parameter distributions ( $\mu$ : mean;  $\sigma$ : standard deviation;  $\alpha$ : shape parameter;  $\beta$ : scale parameter).

et al., 2014). The distributions of PROSPECT parameters were estimated 399 from seventeen independent data sets made available by Féret et al. (2011); 400 Féret, personal communication. They include a wide range of leaf spec-401 tral, chemical, and structural properties, i.e., 1417 leaves corresponding to 402 about 120 different species from various growing conditions and develop-403 mental stages. Note that  $C_{ab}$ ,  $C_{cx}$ ,  $C_w$  and  $C_m$  data were obtained in a 404 destructive way, whereas N data were obtained from PROSPECT inversion 405 on DHR data. It can be shown that these data are well described by Gamma 406 distributions (p < 0.001). Using such distributions (instead of normal ones) 40 prevented us from generating samples with negative content values. Regard-408 ing brown pigments, we assumed that leaves under study were green so  $C_{bp}$ 409 was set to zero. Finally,  $\theta_i$  and  $b_{spec}$  distributions were retrieved from the 410 estimation results presented in Section 4 using a Gamma distribution for  $\theta_i$ 411 and a normal distribution for  $b_{spec}$  (not shown). The characteristics of all of 412 these distributions are presented in Table 4, where the shape parameter  $\alpha$ 413

and the scale parameter  $\beta$  of the Gamma distribution were given by their maximum likelihood estimates. Note that two  $b_{spec}$  distributions were used for the two spectral domains. Importantly, the covariance between parameters could not be considered when generating the samples. Consequently, the actual influences of  $C_{ab}$  and  $C_{cx}$  are likely to be slightly different, both parameters being highly correlated (Féret et al., 2008).

For each EFAST run, 5000 leaf reflectance spectra were therefore simulated
using PROSPECT and PROCOSINE (Eq. 20) so as to compute first-order
indices and interactions. Average indices were finally computed over 15 runs.

#### 423 4. Results and discussion

# 424 4.1. Sensitivity analysis

In Figure 3, we compare the first-order indices and interactions obtained 425 with PROSPECT and PROCOSINE over the VNIR and SWIR ranges. Fig. 3.a 426 and Fig. 3.b reveal the same features already observed in previous studies 42 using other methods and/or models (Jacquemoud & Baret, 1990; Jacque-428 moud et al., 2009; Bacour et al., 2001, 2002; Bowyer & Danson, 2004). In 429 the visible range (400-730 nm), photosynthetic pigments (i.e., chlorophyll 430 and carotenoids) drive most of the reflectance variability. Between 400 and 431 525 nm where the carotenoid absorption is the strongest (Féret et al., 2008), 432 the contributions of  $C_{ab}$  and  $C_{cx}$  are similar in magnitude and range from 433 20 to 40%. Between 525 and 730 nm, reflectance mainly depends on  $C_{ab}$ , its 434 contribution ranging from 40 to 90%. The influence of interactions is higher 435 in strong absorption regions, which means that the effects of other param-436 eters depend on  $C_{ab}$  and  $C_{cx}$  values. For example, the relative increase in 437



Figure 3: First-order sensitivity indices and interactions for (a) PROSPECT in the VNIR range, (b) PROSPECT in the SWIR range, (c) PROCOSINE in the VNIR range, and (d) PROCOSINE in the SWIR range ( $\theta_s = 26^o$ ).

reflectance due an increase in N (reflecting higher scattering within the leaf
internal structure) will be high in case of low absorption and low in case of
strong absorption.

In the NIR plateau, variation in reflectance is mainly produced by variation 441 in leaf structure (80%) and leaf mass per area (14%) through scattering pro-442 cesses (Knyazikhin et al., 2013). In the SWIR range, only leaf structure, 443 equivalent water thickness and leaf mass per area have significant contribu-444 tions. In particular,  $C_w$  strongly influences reflectance in the water absorp-445 tion peaks located around 1450 and 1950 nm (about 75%), whereas variation 446 in  $C_m$  has a significant contribution around 1720 and 2250 nm (resp. 24%) 44 and 30%). 448

449

Taking into account BRDF effects and leaf orientation through the  $b_{spec}$ and  $\theta_i$  parameters within the PROCOSINE model modifies the reflectance sensitivity as shown in Figure 3.c and Figure 3.d. Compared with PROSPECT sensitivity analysis, the overall contributions of PROSPECT parameters are mostly similar in shape but still, they decrease to account for variance in  $b_{spec}$  and  $\theta_i$ . For example, the  $C_{ab}$  contribution at around 550 nm decreases from 90 to 70%.

The contributions of  $b_{spec}$  and  $\theta_i$  are quite different. Overall, variance in  $b_{spec}$  highly influences reflectance in strong absorption regions (both due to  $C_{ab}$  and  $C_w$ ), accounting for up to 90% near 400 nm and 75% near 1930 and 2500 nm. In these regions, the diffuse part of reflectance is very low so the influence of the surface-reflected flux (that does not interact with the leaf volume) dominates. Interestingly, an analogy can be made with high-

resolution water remote sensing, in that the sun glint (i.e., the amount of flux directly reflected at the water surface) is usually estimated in the NIR region, where the water-leaving signal is negligible because of strong water absorption (Hochberg et al., 2003). Overall, the  $b_{spec}$  contribution is always greater than 15% between 400 and 2500 nm, thereby indicating that this parameter should not be neglected when dealing with close-range hyperspectral images.

470

The contribution of the incident angle  $\theta_i$  significantly varies over the whole 471 spectral domain. It mostly affects reflectance in the NIR plateau, accounting 472 for about 30% of the variance of the PROCOSINE output. Conversely, its 473 influence is much weaker in the visible range, where its contribution does 474 not exceed 5%, as well as in water absorption regions. Generally, because 47 it affects the model through a multiplicative term (see Eq. 20 and Eq. 21), 476 the spectral profile of its contribution is similar to a common leaf spectral 47 signature: the higher the reflectance, the higher its contribution. Interest-478 ingly, this profile is also similar to the contribution of the average leaf angle 479 (ALA) to the PROSAIL model (Jacquemoud et al., 2009). In the latter case, 480 ALA has more influence at weakly absorbing wavelengths because the effect 481 of multiple scattering within the canopy is stronger (Knyazikhin et al., 2013). 482 483

To summarize, this sensitivity analysis shows that both  $b_{spec}$  and  $\theta_i$  significantly affect the measured signal and definitively have to be taken into account in the case of close-range imaging spectroscopy.

#### 487 4.2. Quantitative assessment of model inversion

The performances of model inversion were quantitatively assessed both in terms of spectral fitting and parameter retrieval. Note that we had only reference measurements integrated over one (for  $C_{ab}$ ) or several (for  $C_w$  and  $C_m$ ) leaf disk(s) of a few square centimeters. As a result, in this section, the means and standard deviations of  $C_{ab}$ ,  $C_w$  and  $C_m$  estimated values were computed from the values estimated within the corresponding leaf disk(s).

# 494 4.2.1. PROCOSINE spectral accuracy

We first quantified how accurate was PROCOSINE in fitting the pseudo-BRF and radiance measurements retrieved at the pixel level. In Fig. 4, we show some fitting results obtained with an ivy leaf both for the VNIR and SWIR ranges, this leaf surface being non-Lambertian and non-regular.

Overall, strong agreements were obtained between measured and simulated 499 spectra in the two ranges (RMSE < 4%). As expected, high  $b_{spec}$  values were 500 retrieved in areas affected by specular reflection, and high  $\theta_i$  values were 50 retrieved where the light incident angle was high. Compared with the VNIR 502 range, the obtained RMSE were about twice higher for the SWIR range. 503 This is in agreement with the mismodeling of specular reflection in the SWIR 504 range mentioned in Section 2.2.1 and discussed further in Section 4.2.4. These 505 results thus demonstrate the accuracy of PROCOSINE in accounting for the 506 spectral variability induced by BRDF effects and leaf orientation, especially 507 in the VNIR range. 508



Figure 4: Fitting results obtained for the VNIR range (a-c) and the SWIR range (d-f) using the pseudo-BRF model (b,e) and the radiance model (c,f). Solid (resp. dashed) lines correspond to measurements (resp. simulations). Blue curves correspond to areas strongly affected by specular reflection, while red curves correspond to areas characterized by a high incident angle.



Figure 5:  $C_{ab}$  estimation results (mean +/- standard deviation) obtained with PROSPECT (blue), the pseudo-BRF based PROCOSINE model (orange), and the radiance-based PROCOSINE model (green) and with  $\bar{\theta}_i = 20^o$  (a-c),  $\bar{\theta}_i = 0^o$  (d-f) and  $\bar{\theta}_i = 40^o$  (g-i). The R<sup>2</sup> and RMSE values are computed for actual  $C_{ab}$  values lower than  $40 \ \mu \text{g.cm}^{-2}$  and are given in parentheses.

#### 509 4.2.2. Results of parameter retrievals in the VNIR range

519

As recalled by the sensitivity analysis, the VNIR reflectance is mainly 510 driven by the chlorophyll a+b content. In Fig. 5, we show the means and 511 standard deviations of  $C_{ab}$  estimation obtained for each leaf disk with leaves 512 in horizontal position (Figure 5.a-c) and tilted position (Figure 5.d-i). We 513 compare the results obtained with PROSPECT (in blue), the pseudo-BRF 514 based PROCOSINE model (in orange) and the radiance-based PROCOSINE 515 model (in green). Because of the saturation in the reference measurement 516 (see Section 3.1.2), the RMSE and  $R^2$  values were computed from samples 51 for which the measured  $C_{ab}$  values were lower than 40  $\mu$ g.cm<sup>-2</sup>. 518

On average, when tested with horizontal leaves, the radiance-based PRO-520 COSINE model led to a higher accuracy ( $R^2 = 0.92$ ;  $RMSE = 3.23 \ \mu g.cm^{-2}$ ) 521 than the pseudo-BRF PROCOSINE model ( $R^2 = 0.89$ ;  $RMSE = 3.73 \ \mu g. cm^{-2}$ ) 522 and PROSPECT ( $R^2 = 0.81$ ; RMSE = 4.88  $\mu g.cm^{-2}$ ). Applying the same 523 models to leaves in tilted position decreased the estimation accuracy, how-524 ever to a variable extent. For  $\bar{\theta}_i = 0^{\circ}$ , the radiance-based PROCOSINE 525 model ( $R^2 = 0.93$ ; RMSE = 4.44 µg.cm<sup>-2</sup>) still performed better than the 526 pseudo-BRF based PROCOSINE model ( $R^2 = 0.92$ ;  $RMSE = 4.71 \ \mu g. cm^{-2}$ ) 527 and PROSPECT ( $R^2 = 0.81$ ; RMSE = 6.45 µg.cm<sup>-2</sup>). The same trend was 528 also observed for  $\bar{\theta}_i = 40^\circ$ , the radiance-based PROCOSINE model leading 529 to a better accuracy ( $R^2 = 0.91$ ; RMSE = 3.65  $\mu g.cm^{-2}$ ) than the pseudo-530 BRF based PROCOSINE model ( $R^2 = 0.86$ ; RMSE = 4.63  $\mu$ g.cm<sup>-2</sup>) and 53 PROSPECT ( $R^2 = 0.87$ ; RMSE = 5.87 µg.cm<sup>-2</sup>). 532

533 Overall, both PROCOSINE implementations obtained significantly lower



Figure 6: Histograms of estimated  $\theta_i$  values for every pixel for the VNIR range and the three acquisition configurations ( $\bar{\theta}_i = 0^o$ ,  $\bar{\theta}_i = 20^o$ , and  $\bar{\theta}_i = 40^o$ ): (a) pseudo-BRF based PROCOSINE model, and (b) radiance-based PROCOSINE model.

standard deviations of  $C_{ab}$  estimation than PROSPECT.

Lastly, for  $C_{ab} > 40 \ \mu \text{g.cm}^{-2}$ , model inversion always provided higher  $C_{ab}$ values than those measured with the Dualex.

537

The incident angle estimation within the whole leaves is evaluated in Fig. 6. The results are presented using histograms to account for within-leaf variability of leaf orientation. For both model implementations, we represent the distributions of  $\theta_i$  values estimated for every pixel for the three acquisition configurations (i.e., average incident angles  $\bar{\theta}_i$  of 0°, 20°, and 40°).

Surprisingly, strong differences were observed between both model inversions. On the one hand, the pseudo-BRF based model gave poor estimation results with estimated  $\bar{\theta}_i$  of 3.3°, 5.1° and 11.7° (and the same estimated distribution mode, i.e., 2.4°) for  $\bar{\theta}_i = 0^\circ$ ,  $\bar{\theta}_i = 20^\circ$ , and  $\bar{\theta}_i = 40^\circ$  respectively. On the other hand, the radiance-based model gave better estimation results with estimated  $\bar{\theta}_i$  of 9.7°, 16.9° and 19.6° (and estimated distribution modes of 6.3°, 14.8°

- and 14.8°) for  $\bar{\theta}_i = 0^\circ$ ,  $\bar{\theta}_i = 20^\circ$ , and  $\bar{\theta}_i = 40^\circ$  respectively.
- <sup>550</sup> It is worth noting that poorer angle estimation results were generally obtained
- <sup>551</sup> for bamboo leaves (results not shown) with estimated distribution modes of
- <sup>552</sup> 15.4°, 28.6° and 28.6°) for  $\bar{\theta}_i = 0^\circ$ ,  $\bar{\theta}_i = 20^\circ$ , and  $\bar{\theta}_i = 40^\circ$  respectively.

# 553 4.2.3. Results of parameter retrievals in the SWIR range

Regarding PROSPECT original parameters, variation in SWIR reflectance is mainly produced by variation in equivalent water thickness, leaf mass per area and leaf structure.

In Fig. 7, we show the means and standard deviations of  $C_w$  estimation 55 obtained with leaves in horizontal position (Fig. 7.a-c) and in tilted posi-558 tion (Fig. 7.d-i). For horizontal leaves, PROCOSINE performed better than 559 PROSPECT in terms of  $R^2$  ( $R^2 = 0.91$  for PROSPECT,  $R^2 = 0.93$  for 560 the pseudo-BRF based PROCOSINE model and  $R^2 = 0.94$  for the radiance-56 based PROCOSINE model), but worse in terms of RMSE (RMSE = 0.0016 cm, 562 RMSE = 0.0083 cm and RMSE = 0.0025 cm resp.). However, the PRO-563 COSINE performances remained mostly unchanged when applied to tilted 564 leaves, while PROSPECT obtained poorer performances, either for  $\bar{\theta}_i = 10^o$ 56!

(a 125% increase in RMSE) or  $\bar{\theta}_i = 50^o$  (a 15% decrease in R<sup>2</sup>).

The RMSE values obtained with PROCOSINE were primarily due to a systematic bias, the  $R^2$  values being higher than 0.91 for the three acquisition configurations. This bias was more pronounced for the pseudo-BRF based model, and led to a systematic overestimation of  $C_w$ .

Lastly, similarly to  $C_{ab}$  estimation, PROCOSINE obtained lower standard deviations of  $C_w$  estimation than PROSPECT, especially for tilted leaves.



Figure 7:  $C_w$  estimation results (mean +/- standard deviation) obtained with PROSPECT (blue), the pseudo-BRF based PROCOSINE model (orange), and the radiance-based PRO-COSINE model (green) and with  $\bar{\theta}_i = 30^o$  (a-c),  $\bar{\theta}_i = 10^o$  (d-f) and  $\bar{\theta}_i = 50^o$  (g-i). R<sup>2</sup> and RMSE values are given in parentheses.



Figure 8:  $C_m$  estimation results (mean +/- standard deviation) obtained with PROSPECT (blue), the pseudo-BRF based PROCOSINE model (orange), and the radiance-based PRO-COSINE model (green) and with  $\bar{\theta}_i = 30^o$  (a-c),  $\bar{\theta}_i = 10^o$  (d-f) and  $\bar{\theta}_i = 50^o$  (g-i). R<sup>2</sup> and RMSE values are given in parentheses.



Figure 9: Histograms of estimated  $\theta_i$  values in every pixel for the SWIR range and the three acquisition configurations ( $\bar{\theta}_i = 10^o$ ,  $\bar{\theta}_i = 30^o$ , and  $\bar{\theta}_i = 50^o$ ): (a) pseudo-BRF based PROCOSINE model, and (b) radiance-based PROCOSINE model.

The  $C_m$  retrieval results are presented in Fig. 8 in a similar fashion to  $C_w$ . 574 The radiance-based PROCOSINE model gave significantly lower RMSE than 575 the pseudo-BRF based PROCOSINE model and PROSPECT, i.e., RMSE =576  $0.0013 \text{ g.cm}^{-2}$ , RMSE =  $0.0032 \text{ g.cm}^{-2}$ , and RMSE =  $0.0024 \text{ g.cm}^{-2}$  respec-577 tively on average for the three acquisition configurations. The PROCOSINE 578 performances weakly depended on leaf position, whereas the  $R^2$  dropped 579 from 0.89 for  $\bar{\theta}_i = 10^o$  and  $\bar{\theta}_i = 30^o$ , to 0.30 for  $\bar{\theta}_i = 50^o$  when inverting only 580 PROSPECT. For such high incident angles, the uncertainty of  $C_m$  estimation 583 was much higher with PROSPECT than with PROCOSINE. 582 Lastly,  $C_m$  was generally underestimated by PROSPECT and overestimated 583

Lastly,  $C_m$  was generally underestimated by PROSPECT and overestimated by the pseudo-BRF based PROCOSINE model.

585

The two PROCOSINE inversions were also compared based on  $\theta_i$  estimation results in Fig. 9, in which we represent the histograms of estimated  $\theta_i$  distributions. As expected, in both cases, the highest (resp. the lowest)

angles were mostly retrieved from the  $\bar{\theta}_i = 50^{\circ}$  (resp.  $\bar{\theta}_i = 10^{\circ}$ ) configuration, the dispersions around the mean values being due to the variation in leaf orientation.  $\theta_i$  was more accurately predicted using the radiance-based model since the estimated  $\bar{\theta}_i$  were 19.7°, 27.7° and 36.4° for  $\bar{\theta}_i = 10^{\circ}$ ,  $\bar{\theta}_i = 30^{\circ}$ , and  $\bar{\theta}_i = 50^{\circ}$  respectively. The pseudo-BRF based model globally overestimated  $\theta_i$  since the estimated  $\bar{\theta}_i$  were 38.0°, 47.2° and 53.0° for  $\bar{\theta}_i = 10^{\circ}$ ,  $\bar{\theta}_i = 30^{\circ}$ , and  $\bar{\theta}_i = 50^{\circ}$  respectively.

Similarly to the VNIR range, poorer estimation results were generally obtained for bamboo leaves (results not shown). For example, the radiancebased model led to estimated  $\bar{\theta}_i$  of 38.0°, 43.4° and 47.0° for  $\bar{\theta}_i = 10^\circ$ ,  $\bar{\theta}_i = 30^\circ$ , and  $\bar{\theta}_i = 50^\circ$  respectively.

## 600 4.2.4. Discussion about parameter retrievals

*Estimation of chlorophyll content.* In the VNIR range, both PROCOSINE 601 implementations performed better than PROSPECT in retrieving  $C_{ab}$ . For 602 leaves in horizontal position, the 34% improvement in RMSE when using the 603 radiance-based PROCOSINE model instead of PROSPECT is likely to be 604 due mainly to the modeling of BRDF effects. Not taking them into account 605 leads to a greater uncertainty as shown through the estimation standard devi-606 ations computed within each leaf disk. For example, as illustrated in Fig. 5.a 60 with the sample corresponding to an actual mean value of 53  $\mu$ g.cm<sup>-2</sup>, a 608 local BRDF effect induces an overall increase in reflectance, which is misin-609 terpreted by PROSPECT as a decrease in  $C_{ab}$ . This result confirms one of the 610 conclusions drawn from the sensitivity analysis, which has already showed 61 that  $b_{spec}$  significantly affects leaf close-range hyperspectral measurements. 612 The difference between PROCOSINE and PROSPECT was even greater 613

when considering leaves in tilted position, for which the modeling of leaf 614 inclination was more important. In particular, for the highest incident angle 615  $(\theta_i = 40^\circ)$ , both the modeling of BRDF effects and leaf orientation within 616 the radiance-based PROCOSINE model led to an actual 38% improvement 617 over PROSPECT. It is worth noting that taking  $\theta_i$  into account improves 618 the  $C_{ab}$  estimation results even if  $C_{ab}$  is mainly retrieved between 400 and 619 750 nm, in which the effect of  $\theta_i$  is lower (see Fig. 3.c). In fact, the difference 620 in retrieval performance in VNIR between PROSPECT and PROCOSINE is 62 even greater for N leaf structure parameter that mainly affects reflectance 622 in the NIR plateau, where both  $\theta_i$  and  $b_{spec}$  have a strong influence on re-623 flectance (N maps are only shown for the SWIR range, see Fig. 12). 624

The PROCOSINE inversion performed well compared with the accuracy pro-625 vided by the Dualex manufacturer, i.e.,  $RMSE = 5 \ \mu g.cm^{-2}$  (Cerovic et al., 626 2012), especially considering that spectral measurements are affected by ex-62 tra variability and that the method is based on reflectance, which is known to 628 be less sensitive to  $C_{ab}$  than transmittance (Baret & Fourty, 1997b). Impor-629 tantly, the apparent  $C_{ab}$  overestimation for  $C_{ab} > 40 \ \mu g.cm^{-2}$  was rather due 630 to the saturation in the reference measurement (see Section 3.1.2), as also 631 suggested by the similar trend observed for both PROSPECT and PRO-632 COSINE. Further experiments conducted on hyperspectral data associated 633 with laboratory extraction based measurements of pigment contents (includ-634 ing  $C_{cx}$  would, however, be interesting to fully characterize the pigment 635 retrieval. 636

<sup>637</sup> The main difference between both PROCOSINE inversions arose for high <sup>638</sup> incident angles, since the RMSE decreased by 21% when using the radiance-

based model. This result confirms that this implementation better handles
variation in leaf orientation as displayed in Fig. 6.

Estimation of equivalent water thickness and leaf mass per area. Somewhat 641 different observations could be made from the SWIR range. In most cases, 642 the retrievals of  $C_w$  and  $C_m$  resulted in lower RMSE when using the radiance-643 based PROCOSINE model. In particular, the  $C_m$  estimation was very accu-644 rate even if  $C_m$  is not the most influential parameter in this spectral domain 645 (see Fig. 3.d). The poor  $\mathbb{R}^2$  value and very high standard deviations obtained 646 with PROSPECT and  $\bar{\theta}_i = 50^{\circ}$  again demonstrate the need for accounting 64 for BRDF effects and leaf orientation, especially when the targeted parame-648 ter does not have a strong influence on reflectance. 649

650

However, as recalled in Section 2.2.1, BRDF effects are not properly taken 651 into account for the SWIR range because, unlike the VNIR range,  $b_{spec}$  de-652 pends on wavelength. Indeed, the BRDF directional component depends on 653 the leaf refractive index (Bousquet et al., 2005), whose imaginary part is 654 proportional to absorption (Born & Wolf, 1980). Especially at the far end 655 of the SWIR range, water absorption is so strong (Hale & Querry, 1973) 656 that the imaginary part of the leaf refractive index is no longer negligible 65 compared with the real part (Gerber et al., 2011). This may explain why 658 PROSPECT is more accurate than PROCOSINE in retrieving  $C_w$  on leaves 659 in horizontal position. Presumably, PROCOSINE systematically overesti-660 mates  $C_w$  to mimic the decrease of the leaf refractive index (Féret et al., 663 2008). The compensation between  $C_w$  and  $b_{spec}$  allows the proposed models 662 to be adjusted to the SWIR range and to obtain better estimation results 663

for other PROSPECT parameters such as  $C_m$ . For leaves in tilted position, the influence of leaf orientation, whose modeling does not depend on wavelength, again makes the radiance-based PROCOSINE model more accurate than PROSPECT.

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Importantly, the high  $R^2$  values obtained with PROCOSINE for  $C_w$  and  $C_m$  retrievals make it possible to calibrate strong linear relationships between the actual values and the estimated values. Indeed, in every case, the obtained RMSE is driven more by the estimation bias than by the variance. As carried out by Cheng et al. (2011), applying such an indirect retrieval could correct this bias and significantly enhance the estimation results obtained with a given experimental setup.

Angle estimation. Both in the VNIR and SWIR ranges, the performances of 676 PROCOSINE weakly depended on leaf position. This tends to prove that 671 non-regular surfaces can be handled properly by introducing the  $\theta_i$  parame-678 ter. However, some clear differences arose between pseudo-BRF and radiance 679 inversions. Overall, inverting the radiance-based model provided the best re-680 sults, the strongest difference between both ranges lying in  $\theta_i$  estimation, 68 especially in the VNIR range.  $\theta_i$  was indeed better retrieved using radiance-682 based inversion, the  $\theta_i$  underestimation for high incident angles and both 683 ranges being presumably due to the assumption  $\frac{1-\rho_{spec}(\theta_i;2\pi)}{1-\rho_{spec}(0;2\pi)} \approx 1$  in Eq. 20. 684 It could be shown that confounding effects between  $\theta_i$  and N (as well as  $C_m$ ) 685 in the VNIR range) were responsible for poor  $\theta_i$  estimation results obtained 686 through pseudo-BRF inversion. For example, as observed in Fig. 3, both  $\theta_i$ 68 and N have similar contributions to the model output. However, they also 688

have opposite effects, which may lead the inversion process to misinterpret an increase in  $\theta_i$  as a decrease in leaf structure N. Therefore, in the VNIR (resp. SWIR) range, this model compensates  $\theta_i$  underestimation (overestimation) by N underestimation (overestimation).

On the other hand, several assumptions can be made regarding the good 693 performances obtained by radiance-based inversion. First, this may be due 694 to the noise level in the spectral measurements: as the ratio of two radi-695 ance spectra is noisier than both radiance spectra independently, retrieved 696 pseudo-BRF spectra thus have a lower signal-to-noise ratio than originally 69 measured radiance spectra. This problem is critical near 400 nm and in the 698 NIR plateau where the sensitivity of the VNIR camera is lower compared 699 with most of the visible range (see Fig. 4). This emphasizes the necessity 700 of acquiring spectral measurements as clean as possible. Alternatively, such 70 differences in the inversion performances may be due to the numerical imple-702 mentation of the inversion process (e.g., through the considered cost function, 703 optimization algorithm or initialization). Further investigation is therefore 704 needed to fully optimize the PROCOSINE inversion. 705

706

Finally, the poorer angle estimation results obtained with bamboo leaves were likely to be due to the azimuthally anisotropic roughness properties of monocotyledon leaves, that mainly originate from the longitudinal orientation of veins (Comar et al., 2012, 2014). Unlike regular surfaces for which the BRF is azimuthally symmetric, such an organized arrangement of the leaf surface leads the specular lobe not to be in the principal plane (Miesch et al., 2002). In this case, it may seem inappropriate to represent the local

leaf inclination at the pixel level using only a single mean angle, especially
because the image spatial resolution is comparable to the inter-vein distance
for monocotyledons, i.e., a few hundred micrometers (Comar et al., 2014).
However, other estimation results presented in this paper strongly suggest
that this does not affect the retrievals of leaf biochemical properties.

#### 719 4.3. Leaf parameter mapping

Hyperspectral imaging allowed us to obtain high-resolution maps of model parameters by inverting the model for each pixel. Compared with the results obtained from estimated values averaged within one or several leaf disk(s) (each of which contains several hundreds of pixels), such maps provide a deeper insight in how these effects actually affect the estimation process.

In Fig. 10 and Fig. 11, we show some estimated maps obtained using PROSPECT 725 and the radiance-based PROCOSINE model respectively, the radiance-based 726 inversion performing better than the pseudo-BRF inversion as seen in Sec-72 tion 4.2. The considered bay laurel leaf was chosen due to its strong non 728 Lambertian behavior and to the presence of a large range of  $C_{ab}$  and  $C_{bp}$ 729 The actual chlorophyll content in the greenest area was close to values. 730 40  $\mu$ g.cm<sup>-2</sup>, while the equivalent water thickness and leaf mass per area were 73 0.0088 cm and 0.0099 g.cm<sup>-2</sup> respectively. 732

On the one hand, as observed in Fig. 10, PROSPECT estimation was strongly affected by BRDF effects both in the VNIR and SWIR ranges. This increase in reflectance is not taken into account by PROSPECT, which resulted in some compensations during the inversion, here corresponding to an increase in  $C_{bp}$  and decreases in  $C_{ab}$  (as already mentioned in Section 4.2.2),  $C_w$  and  $C_m$ . On the other hand, in Fig. 11, we show that these BRDF effects were



Figure 10: Estimated maps obtained using PROSPECT in the VNIR (a-c) and SWIR (d-f) ranges: (a) true color composite image, (b)  $C_{ab}$ , (c)  $C_{bp}$ , (d) false color composite image (using bands 1458 nm, 2202 nm and 1662 nm), (e)  $C_w$ , (f)  $C_m$ .

<sup>739</sup> correctly interpreted as local increases in  $b_{spec}$  within the PROCOSINE in-<sup>740</sup> version. Accurate descriptions of the actual regular leaf orientation were also <sup>741</sup> obtained through homogeneous  $\theta_i$  maps and average  $\theta_i$  of 15° and 30° for the <sup>742</sup> VNIR and SWIR ranges respectively.

<sup>743</sup> Modeling such extra variability therefore allowed us to obtain consistent maps <sup>744</sup> of foliar content. In the VNIR range, the highest  $C_{ab}$  values were obtained <sup>745</sup> in the greenest parts with values close to 40  $\mu$ g.cm<sup>-2</sup>, while very low chloro-<sup>746</sup> phyll contents were retrieved in senescent parts, especially in the necrotic <sup>747</sup> area on the top (Fig. 11.b). This latter area was also exhibiting a high con-<sup>748</sup> tent in brown pigments as shown in Fig. 11.c, thereby proving the reliability



Figure 11: Estimated maps obtained using the radiance-based PROCOSINE model in the VNIR (a-e) and SWIR (f-j) ranges: (a) true color composite image, (b)  $C_{ab}$ , (c)  $C_{bp}$ , (d)  $b_{spec}$ , (e)  $\theta_i$ , (f) false color composite image (using bands 1458 nm, 2202 nm and 1662 nm), (g)  $C_w$ , (h)  $C_m$ , (i)  $b_{spec}$ , (j)  $\theta_i$ .

<sup>749</sup> of PROSPECT for retrieving pigments.

<sup>750</sup> Consistent maps were obtained in the SWIR range as well. As expected, <sup>751</sup> veins were found to contain a lot of water, unlike the upper part where <sup>752</sup> necrosis was causing a strong water loss (Fig. 11.g). Although being a bit <sup>753</sup> more affected than  $C_w$  by mismodeled BRDF effects,  $C_m$  was estimated more <sup>754</sup> accurately than  $C_w$  since both  $C_w$  and  $C_m$  average estimated values were close <sup>755</sup> to 0.011 g.cm<sup>-2</sup>.

In particular, these maps are very appealing for identifying plant diseases at leaf scale. As described by Mahlein et al. (2013), different diseases may lead to different symptoms that can be characterized by local changes in optical properties, e.g., a higher chlorophyll/carotenoid ratio for sugar beet rust, or necrosis for *Cercospora* leaf spot. Therefore, inverting PROCOSINE based on VNIR and SWIR hyperspectral images of the same leaf offers very interesting perspectives for early detection of many plant diseases.

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Finally, in Fig. 12, we provide a last example that again demonstrates the 764 potential of PROCOSINE in the SWIR range when tested with a sugar beet 765 leaf characterized by high  $C_w$  ( $C_w = 0.0355$  cm) and low  $C_m$  ( $C_m = 0.0040$  g.cm<sup>-2</sup>) 766 values, and by a strongly non-regular and non-Lambertian leaf surface. Even 76 if PROSPECT obtained better results when considering estimated values av-768 eraged over the five sampled leaf disks ( $\hat{C}_w = 0.0370 \text{ cm}; \hat{C}_m = 0.0032 \text{ g.cm}^{-2}$ ), 769 it also led to highly heterogeneous and inconsistent maps, whose variances 770 obviously did not reflect the actual ones but rather expressed unmodelled 77 variability. Conversely, the PROCOSINE inversion led to homogeneous and 772 consistent maps, either for leaf structure ( $\hat{N} = 1.30$ ; to compare with 773



Figure 12: Estimated maps obtained in the SWIR range using the radiance-based PRO-COSINE model (b-f) and PROSPECT (g-i): (a) false color composite image (using bands 1458 nm, 2202 nm and 1662 nm), (b)  $b_{spec}$ , (c)  $\theta_i$ , (d) N, (e)  $C_w$ , (f)  $C_m$ , (g) N, (h)  $C_w$ , (i)  $C_m$ .

the mean value of 1.225 provided by Jacquemoud et al. (1996) for the same 774 species), equivalent water thickness ( $\widehat{C}_w~=~0.042~{\rm cm})$  and leaf mass per area 775  $(\widehat{C}_m = 0.0052 \text{ g.cm}^{-2})$ . In particular, the strongly non regular leaf orienta-776 tion was greatly retrieved through the estimated  $\theta_i$  map (Fig. 12.c): regions 777 with low estimated  $\theta_i$  were indeed facing the light source while regions with 778 high estimated  $\theta_i$  were facing the opposite side (note that shadows were inter-779 preted as high  $\theta_i$  values). Interestingly, most imaging techniques allowing the 780 retrieval of leaf (or even plant) orientation are either based on depth imaging 78 systems (Chéné et al., 2012) or on 3D models built from multi-angular obser-782 vations using stereovision (Lati et al., 2013) or photogrammetry (Jay et al., 783 2015). In comparison, it is worth noting that in this study, the retrieval of 784 leaf orientation only necessitates a single-angular observation and is based 785 on spectral information only. 786

#### 787 5. Conclusions and perspectives

In this study, we propose a physically-based model that allows for ap-788 plying rigorously a DHR model of leaf optical properties to pseudo-BRF 789 hyperspectral (or multispectral) images acquired with close-range imaging 790 spectroscopy. The proposed COSINE model describes the spectral variabil-79 ity caused by variable BRDF effects and leaf orientation, that, depending 792 on leaf surface, can make the acquired pseudo-BRF measurements very dif-793 ferent from DHR measurements. In this paper, COSINE is coupled with 794 PROSPECT and the numerical inversion of the resulting PROCOSINE model 795 led to accurate leaf-level mappings of foliar content and above leaf surface 796 properties, both in the VNIR and SWIR ranges. 79



Figure 13: Use of the PROCOSINE model for image pretreatment in the VNIR (a-c) range: (a) DHR image reconstructed with PROSPECT and estimated parameters, (b) *SBRI* map (Mahlein et al., 2013) obtained with the original image, and (c) *SBRI* map (Mahlein et al., 2013) obtained with the reconstructed image.

Besides avoiding the need for hemispherical measurements, the proposed ap-798 proach allows the non-destructive biochemical characterization of small leaves 799 thanks to the sub-millimeter resolution of hyperspectral images. Potentially, 800 it could represent a practical solution for optical characterization of needles, 803 whose optical properties were found to be well described by PROSPECT 802 (Moorthy et al., 2008) (usual needle optical measurements involving using 803 complex experimental setups to handle irregularities in size, shape and cur-804 vature). As previously mentioned, it can also be combined with other leaf 805 DHR models such as LIBERTY (Dawson et al., 1998). 806

The accurate retrieval of  $C_m$  makes it possible to derive mass-based quantities from surface-based quantities. In particular, strong correlations ( $\mathbb{R}^2 > 0.85$ ) were obtained for the estimation of Gravimetric Water Content (being expressed as  $C_w/C_m$ ), which is an important indicator for fire risk modeling (Chuvieco et al., 2004).

Potential applications also include the use of PROCOSINE as a pretreatment for further processing. To illustrate, in Fig. 13.a, we show a DHR image reconstructed by running PROSPECT in a forward mode with parameters previously estimated with the radiance-based PROCOSINE model

(the original image is presented in Fig. 10). For example, computing spectral
indices designed for plant disease identification based on this cleaned image
is much more reliable to detect these diseases at early infection stages, especially when these indices are based on wavelengths strongly affected by
BRDF effects, e.g., the SBRI (Mahlein et al., 2013). Alternatively, PROCOSINE could allow the design of spectral indices adapted to close-range
imaging spectroscopy, similarly to Féret et al. (2011).

Further investigation is however needed to properly model the specular com-823 ponent in the SWIR range. In this case, the effect of water absorption on 824 leaf refractive index should be considered to reliably model the wavelength-82 dependency of  $b_{spec}$  parameter. Also, confounding effects between PROCO-826 SINE parameters (e.g.,  $N, \theta_i$  and  $C_m$  in the VNIR range) should be studied 82 more deeply by optimizing the numerical implementation of the iterative op-828 timization or by considering regularization strategies as reviewed by Baret 829 & Buis (2008) and Verrelst et al. (2015), e.g., by using prior knowledge to 830 constrain some model variables, or by generating a look-up table and aver-831 aging the N best solutions. As noted in the discussion, a more exhaustive 832 assessment of PROCOSINE should also be performed over a larger data set 833 encompassing a wider range of pigment, water and dry matter contents prop-834 erly measured using laboratory extraction methods. This would allow us to 835 fully validate the proposed model. Lastly, it is worth mentioning that the 836 use of COSINE based on images acquired under outdoor conditions requires 83 assuming that diffuse illumination (coming from either the sky and/or the 838 surrounding terrain) is negligible compared with direct sunlight. We are 839 currently working towards an improvement of COSINE to account for these 840

influences within the modeling, thus transforming the BRF-based model into
a hemispherical-directional reflectance factor based model. This would allow
processing spatially-resolved data acquired from near-ground remote sensing,
e.g., from a tower or low flying unmanned aerial vehicle.

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